Chemical substance, material, product, goods, waste: a changing ontology

Chemical Substance, Material, Product, Goods, Waste: a Changing Ontology

Elena Ghibaudi [1,*], *Luigi Cerruti* [2]

[1] Dept. of Chemistry, University of Torino, Via Giuria 7, I-10125, Torino, Italy
[2] Independent researcher, Viale delle acacie 12, I-10148, Vinovo (TO), Italy; E-mail: lcerruti00@gmail.com
***** Author to whom correspondence should be addressed; E-mail: elena.ghibaudi@unito.it; Tel.: +39-(0)11-6707951; Fax: +39-(0)11-6707855.

Abstract

A chemical substance (CS) is instantiated in the material world by a number of quantities of such substance (QCSs), placed in different locations. A change of location implies a change in the net of relationships entertained by the QCS with the region wherein it is found. This fact entails changes of the ontogical status of the CS, as this is not fully determined by the inherent features of the CS and includes a relevant relational contribution.

In order to demonstrate this thesis, we have chosen to analyse the status of quantities of a same CS that are synchronically located in different spacetime regions: a synthetic lab, a lab where the QCS is turned into a material, an industrial plant, the market where the QCS gets a price and a dump waste where the QCS is discarded, respectively:

Chemical substance ⇨ material ⇨ (industrial) product ⇨ goods ⇨ waste

The use of first-order predicate logic, mereology and locative logic allows carrying out a regimentation process that highlights the ontological commitments implied by the formal expressions through which each element of the aforementioned series can be described. The presence of relational properties discloses the systemic nature of the CS instantiated within a spacetime region. The implications of such an aspect are discussed.

Keywords

Chemical substance; predicate logic; locative logic; mereology; regimentation; chemical ontologies

Introduction

In the final chapter of the *Periodic System*, Primo Levi describes the vicissitudes of a Carbon atom that moves from its initial location - a piece of limestone estracted in the far 1840 - to a consecutive number of molecules, such as carbon dioxide, glucose, lactic acid, again carbon dioxide, cellulose, chitin, still carbon dioxide, a protein, and finally an aminoacid that enters a cell belonging to Levi's brain. Whenever the carbon atom is not free of flying in the air within a CO_2 unit, the molecules it stays in are involved in the most varied physiological processes in men, plants and animals, so that Levi defines such atom as "ex-drinker, ex-cedar, ex-wood worm" (Levi 1984, p. 231). Levi's literary virtuosity enhances the changeable ontological texture of the carbon atom that is promptly perceived by chemists. These lines conceal a philosophical suggestion that deserves to be caught: is it possible to switch from the natural language of narrative to a formal language, able to translate and formalize the ontological changes undergone by a chemical entity along its journey through the material world? This is the purpose of the present work: to highlight (and formalize) the fact that a chemical substance (CS) - instantiated in quantities of chemical substance (QCSs) experiencing distinct locations, each characterized by different networks of relationships with the environment - undergoes ontological changes. In other words, the ontology of a CS shows an insuppressible relational character that may be formally pointed out through the conceptual tools of logic.

As an example, we have chosen to examine the status of distinct quantities of a same chemical substance that are synchronically located in a synthetic lab, a lab where the QCS is turned into a material, an industrial plant, the market where the QCS gets a price and a dump waste where the QCS is discarded,[1] respectively:

Chemical substance ⇨ material ⇨ (industrial) product ⇨ goods ⇨ waste

It must be emphasized that this is a synchronic description of the presence of quantities of a same CS in different locations: in the present context the symbol ⇨ only implies a change of location and not a succession of events.[2]

The aim of this work is twofold, philosophical and methodological. Philosophical in that we intend to examine and discuss the above-written series at the ontological level. Methodological, as we aim to show that the status of a CS instantiated in QCSs placed in the aforementioned locations may be formalized through predicate logic and the regimentation procedure proposed by Quine. We sustain that predicate logic is the simplest available conceptual tool that enables highlighting the ontological commitments concealed by a description. The choice of CSs as the object of our investigation implies taking into account the problems of the whole-parts relationships (CS vs. QCSs) as well as the dynamic relationships between a CS and the region wherein it is instantiated. Hence we exploited mereology and locative logic besides predicate logic.

In the following sections we will describe and discuss the use and application of the aforementioned conceptual tools in the context of this research. This will lead us to draw some conclusions concerning the ontology of CSs.

Regimentation *à la* Quine

As the concept of *ontological change* is central in this work, it is worth specifying its meaning in the present context and expounding the philosophical premises of our research.

Traditionally, ontology is the philosophical study of what exists: the study of the kinds of entities in the real world, and the relationships that these entities bear to one another (Spear 2006).

Amongst the many existing kinds of logic, we have chosen to follow Quine and the privilege he assigns to first-order predicate logic. According to Quine, this is the most suitable instrument for

[1] The four examples of different locations points to the fact that QCSs can have very different masses, running from grams in a chemical lab to thousands of tons in a plant.

[2] The symbol ⇨ was first proposed by the American Society of Mechanical Engineers in 1947, and it is now used in process charts, as "a transportation symbol [that] represents a change of location" (Graham 2004, p. 47).

highlighting the ontological committments concealed in any linguistic register, including common language. Language can be regimented according to first-order predicate logic. Regimentation procedure must be kept as simple as possible: "A *maxim of shallow analysis* prevails: *expose no more logical structure than seems useful* for the deduction or other inquiry at hand" (Quine 1960, p.146).[3]

Quine provides an effective example of regimentation procedures by formalizing a popular observation sentence. With an outright quantification, the sentence "Ravens are Black" becomes:

$$\forall x((x \text{ is a raven}) \rightarrow (x \text{ is black})) \qquad (1)$$

Expression (1) reads as: for any x, if x is a raven, then x is black; other sentences "would be construed similarly, usually by quantifying over times or places" (Quine 1990, pp. 23-36). Apparently, a very simple operation; nevertheless, Quine immediately claims that in his philosophical context (1) is not that trivial:

> "I have insisted down the years that to be is to be the value of a variable. More precisely, what one takes there to be are what one admits as values of one's bound variables".

Quine refers to the renown 'semantical formula' "To be is to be the value of a variable", proposed in 1948 (Quine 1948). Such formula has strong philosophical and epistemic consequences:

> "a theory is committed to those and only those entities to which the bound variables of the theory must be capable of referring in order that the affirmations made in the theory be true."

In this foundational writings, the great American philosopher warns the reader that logical analysis does not disclose 'what really is' in the world; it rather highlights 'what one thinks there is':

> "We look to bound variables in connection with ontology not in order to know what there is, but in order to know what a given remark or doctrine, ours or someone else's, says there is" (Quine 1948).

The polemics raised by this statement induced Quine to confirm almost *verbatim*, in 1970, the position expressed in 1948:

> "What there are, according to a given theory in standard form, are all and only the objects that the variables of quantification are meant in that theory to take as values" (Quine 1970, p.89).

More than 30 years later, Quine still commented his formula as follows:

> "The point has been recognized as obvious and trivial, but it has also been deemed unacceptable, even by readers who share my general philosophical outlook" (Quine 1990).

As compared to other topics of Quine's logical and philosophical thought, the regimentation procedure has been relatively scarcely investigated. Nevertheless, it drew several criticisms to the point that someone ironically wrote about an "armchair paraphrase *à la* Quine" (Glock 2008, p.68).[4] Such criticisms reproach to Quine an 'excess of confidence' on the regimentation of scientific language: critics claim that ontological choices are scientists' own professional duties. We believe that Quine never pretend to intrude upon elseone's field: he just attempted to underline the ontological committments expressed by the language, that are unwittingly taken by 'lay speakers' and are – more or less consciously – taken by scientists.

In the predicate logic x, y, etc. represent variables that may assume all values within a given domain of discourse[5] while *P*, *Q*, etc. are functors with one or more arguments. The expression *P*(x) means that x has the property (expressed by) *P*, or similarly that x is the subject of predicate *P*. If the property expressed by *P* is 'to have mass' and x is a molecule, then *P*(x) is true; if x is a

[3] Italics added by the authors.

[4] Glock is eager for this kind of epithets aimed at Quine (see p. 24 and p. 175).

[5] Intuitively, the domain of discourse is the set of all things we wish to talk about; that is, the set of all objects that we can sensibly assign to a variable.

syllable, then $P(x)$ is false. If the binary functor P means 'to be brother', then $P(x,y)$ means that x and y are brothers and the expression is true if, and only if, x and y are actually brothers. Given a domain of discourse to which x belongs, the existential quantifier ∃ and the universal quantifier ∀ provide the basic formulas:

$\exists x P(x)$ that means that there is at least one x such that $P(x)$ is true, and
$\forall x P(x)$ that means that $P(x)$ is true for all x.

In these formulas, x is the variable bound by quantifiers. If P means 'to be black' and x may assume all values within the domain 'the ravens', the formula $\forall x P(x)$ corresponds to the statement 'all ravens are black'. Hereafter we will introduce other logical operations and their symbols (see Table 2), but the field here outlined was the ground where philosophers of various schools of thought (e.g. rationalists vs. empiricists) fought against each other. This is not surprising as the debate deals with 'what actually exists' and the possible ontological truth of properties and relationships that are assigned to what we believe to exist.

According to Quine's principle of the '*maxim of shallow*' - a kind of modern Occam's logical razor - we have chosen to rely upon the simplest and most straightforward approach that could provide us with the needed tools for achieving the present analysis. In fact, predicate logic - once formulated in a rigorous form - is a flexible and easily-applicable tool, capable of highlighting the properties owned by a CS as well as their change, depending on the context where the CS is instantiated.

Quine's regimentation quantifies over bound variables. Hence, the domain of bound variables - which specifies which values the variable *x* is allowed to take - must be strictly defined because it is critical in determining the truthfulness or falseness of a logic statement. To choose another logic (e.g. second-order logic that quantifies over relations) would have implied an uncontrollable extension of the variables' domain.

Some definitions of chemical substance

Providing a definition of *chemical substance* seems the obvious premise for a reaserch focused on the ontological changes undergone by a CS instantiated in locations as different as a chemical lab or a waste dump. The problem is less trivial than it may seem.

We consider CSs instantiated in a *social environment.* Hence, it is relevant making reference to *public definitions*, not always congruent with the definitions provided by a strictly academic scientific authority. After all, the stringent philosophical analysis by van Brakel has shown the lack of general agreement on the expression 'chemical substance', despite its being crucial for building up chemical ontologies (Van Brakel 2012).

The official IUPAC definition of CS is the following:

> **Def_1:** "Chemical substance: Matter of constant composition best characterized by the entities (molecules, formula units, atoms) it is composed of. Physical properties such as density, refractive index, electric conductivity, melting point etc. characterize the chemical substance" (IUPAC 2014, p. 265).

As chemists, we would consider unacceptable to take material of variable compositions as a CS. Yet, one has to be cautious in disapproving, because the *legal* definition of CS in the 27 States of the European Union is the following:

> **Def_2**: "Substance: a chemical element and its compounds in the natural state or obtained by any manufacturing process, including any *additive* necessary to preserve its stability and any *impurity* deriving from the process used, but excluding any solvent which may be separated without affecting the stability of the substance or changing its composition" (ECA 2011).

These definitions exploit a same term (substance) to designate distinct ontologies. Their comparison highlights that a CS may be identified by referring to distinct material levels (macroscopic, microscopic); in addition, they betray a lack of epistemic awareness. Quite surprisingly, a CS may be either a chemically homogeneous portion of matter or a mixture: in fact, Def_2 admits the presence of *additive* necessary to preserve its stability. Def_2 includes two terms (additive and

impurity) that are usually excluded by the scientific or didactic definition of CS. The legal definition must include those terms because it focuses on CSs that will enter the market; the aim of such choice is clear: identifying the substance for REACH and CLP purposes.[6]

The attitude of the American Chemical Society towards the *identification* of CSs is even looser as compared to the European legislator, albeit more pragmatic and effective. The Web site of the Chemical Abstracts Service (CAS) reports: "CAS Registry contains more than 129 million of unique organic and inorganic chemical substances, such as alloys, coordination compounds, minerals, mixtures, polymers and salts, and more than 67 million sequences" (CAS 2017).[7] American chemists declare the pragmatic aim of an unambiguous identification: "A CAS Registry Number (CASRN) itself has *no inherent chemical significance* but provides an unambiguous way to identify a chemical substance or molecular structure when there are many possible systematic, generic, proprietary or trivial names" (CAS 2017). We have not found a formal definition of substance by the CAS Registry, but an implicit definition is provided by this list:[8]

> **Def**$_3$: "CAS Registry contains a wide variety of substances, including the world's largest collection of:
> Elements
> Organic compounds
> Inorganic compounds
> Metals
> Alloys
> Minerals
> Coordination compounds
> Organometallics
> Isotopes
> Nuclear particles
> Proteins and nucleic acids
> Polymers
> Nonstructurable materials (UVCBs[9])" (CAS 2017).

The list is astonishing in several ways. A first surprise comes from the extreme heterogeneity of the listed species: this reaffirms the generic character assigned by CAS to the term 'chemical substance'. The list includes entities that belong to distinct levels of reality: nuclear particles are besides organic and inorganic compounds; homogeneous and heterogeneous mixtures (alloys and minerals) are associated with simple substances (metals); coordination compounds or polymers are distinct from inorganic and organic species, respectively. Besides, concerning UVCBs included in this list – that certainly do not fall within the disciplinary or didactic definition of CS - OECD remarks that "some CAS number definition are rather narrow, some very broad", but they have the advantage of designating and identifying chemical entities in an unambiguous way (OECD 2014).

The authority of the previous definitions comes from their being proposed by well-recognized public organizations and from their being the expression of a collective agreement. Nonetheless, all of them are troublesome because they stem from the need to face heterogeneous situations (a lab, the market, an industrial plant, etc..). This is not far from the situations described in the present work. At the same time, the regimentation procedure has strict rules and the

[6] REACH is the Regulation for Registration, Evaluation, Authorisation and Restriction of Chemicals. It entered into force on 1st June 2007 to give a framework on chemicals of the European Union (EU); The CLP Regulation (for "Classification, Labelling and Packaging") is a European Union regulation which aligns the European Union system of classification, labelling and packaging chemical substances and mixtures to the Globally Harmonised System, created at the 1992 Rio Conference on Environment and Development. Behind three innocent and purely operational words stays a complex system of classification of risks associated with the use of chemical substances and mixtures.

[7] The Chemical Abstracts Service defines itself as "the world's authority for chemical information".

[8] Definition by list is a process of identifying all the lower-order concepts that make up a higher-order concept (Chaffee 1991).

[9] Unknown, Variable Composition or Biological.

possibility of a univocal designation of a CS is crucial for the application of this kind of logic. Hence, we have chosen to define CSs through their CASRN as it allows a clear-cut identification of the domain of bound variables, as required by first-order logic. Indeed, we are aware of the conceptual problems behind Def_3; nevertheless, we underline that the widespread use of CASRN witnesses an almost universal acknowledgement of Def_3 that has the advantage of being a pragmatic, operational definition that goes well beyond the boundary of a scientific definition.

A logic for natural kinds

Dealing with CSs and their relation with different environments implies taking into account a number of problems that stem from the very nature of such entities, e.g. the whole-part relationship. 'Mass terms' such as 'water' raise a number of questions that have been the object of harsh debates between philosophers and philosophers of science (Kripke1972; Putnam 1973; Needham 2012a; van Brakel 1986) to whom the reader may refer for a broader treatment. We would just like to remind that even recognized experts of language[10] have not been able to grasp the ontological ambiguity of signs and words in chemistry. It was up to philosophers of chemistry to underline repeatedly that, with the symbol H_2O, chemists designate both the molecular species made of 2 hydrogen atoms and 1 oxygen atom and the CS called 'water', exhibiting peculiar properties. Our position agrees with Paul Needham's, who remarks that distinguishing water from ice and steam results in severe logical contradictions. The position shared by the chemists' community may be expressed by formal logic expressions and implies that, if we take 'water (liquid)' and 'H_2O' as predicates, the sentence:

$$\forall x(x \text{ is water (liquid)} \rightarrow x \text{ is } H_2O) \quad (2)$$

is true, whereas the sentence

$$\forall x(x \text{ is } H_2O \rightarrow x \text{ is water (liquid)}) \quad (3)$$

is false (Needham 2012a).

It has been said that a water molecule M_{H2O} and a water droplet W_{drop} belong to distinct ontological levels that may be easily distinguished based on their own properties. If P_{tens} indicates the property of displaying a surface tension, $P_{tens}(W_{drop})$ is true; the corresponding statement "the water droplet has a surface tension" is meaningful and, in specific conditions, it may be complemented by the numerical values of some physical quantities (surface tension, temperature and pressure). By assigning these very same properties to a water molecule, i.e. by stating that $P_{tens}(M_{H2O})$, we get a false expression, corresponding to the statement "a water molecule exhibits surface tension", that is devoid of any physical meaning. Let's now designate as P_{vibr} the property of having a normal mode of vibration: $P_{vibr}(M_{H2O})$ is true and corresponds to the statement "the water molecule has a normal mode of vibration", that may be enriched with "at 3657.1 cm^{-1} and is a symmetric streaching".[11] The formule $P_{vibr}(W_{drop})$ is false, and the statement "the water droplet has a normal mode of vibrations" is devoid of physical meaning. Hence, the logic formalism highlights that the water droplet is the place where some relationships are instantiated, which lack in a water molecule.

Given these premises, and before starting with the regimentation process, it is worth clarifying which kind of logic we intend to use. In recent years, several authors have employed the

[10] Quine, in *Word and Object*, discusses in details the logical gramatics of mass nouns; he wrote: "a mass term in predicative position may be viewed as a general term which is true of each portion of the stuff in question, excluding only the parts too small to count. Thus 'water' and 'sugar', in the role of general terms, are true of each part of the world's water or sugar, down to single molecules but not to atoms" (Quine 1960, p. 89). Immediately after this passage, Quine argue about the sentences "Water is a fluid", "Water is fluid", "Water flows", assigning to water (at the macroscopic level) a property that cannot certainly be assigned to a *single* water molecule (microscopic level).

[11] This frequence refers to the $H_2{}^{16}O$ molecule, one of the eleven water isotopologues (URL: http://www1.lsbu.ac.uk/water/water_vibrational_spectrum.html).

mereologic logic[12] to tackle problems of philosophy of chemistry. An interesting solution, close to our interests, was proposed by Paul Needham, who developed a mereologic and modal treatment applicable to the logical problems of CSs.[13] We will stick to Needham's suggestions and we refer to his works for an in-depth discussion of the principles and applications of his form of mereologic logic. A difference between his and our treatment is that Needham defines the basic variables as *quantities of matter*; we prefer to refer to *quantities of a chemical substance* (QCSs). Our choice is justified by the fact that – as we aim to apply the regimentation process to the language of chemistry – the locution *quantity of chemical substance* seems to fit better, as it makes explicit reference to a physical quantity that is crucial in chemistry, whose unit of measure is the mole. Given this premise, we will now discuss the fundamental mereologic relationships.

Whenever a QCS x is part of a QCS y, we express this relationship through notation $x \subset y$. Notation $x \mid y$ indicates two QCSs that do not share any part with each other. Notation $x \subseteq y$ leads toward an *identity* criterion, which in the mereological context means *to share the same parts*. Identity of two QCSs x, y is formalized as follows:

$$(x \subseteq y \wedge y \subseteq x) \rightarrow (x = y) \quad (4)$$

Axioms of Needham's logic guarantee that for any specific predicate, provided that some QCSs satisfy the predicate ($\exists x P(x)$), there exists only one QCS z that is the *sum* of all QCSs y which satisfies the predicate:

$$\exists x P(x) \rightarrow \exists! z\, (z = \sum y P(y)) \quad (5)$$

Predicates may also have relevant properties. A predicate $P(x)$ is *distributive* if and only if:

$$(P(x) \wedge y \subseteq x) \rightarrow P(y) \quad (6)$$

In other words, a predicate $P(x)$ is *distributive* if and only if any part y of QCS x exhibits the same property *P*.

Quine stated that mass terms such as 'water' have "the semantical property of referring cumulatively: any sum of parts which are water is water" (Quine 1960, p.91). At a formal level, a predicate *Q* is *cumulative* if and only if:

$$\exists x P(x) \wedge \forall x((P(x) \rightarrow Q(x)) \rightarrow Q(\sum x P(x)) \quad (7)$$

$\exists x P(x)$ is an existential statement asserting that there is at least one QCS x that exhibits property *P* (such that $P(x)$); the rest of the expression states that if every QCS with property *P* has also property *Q*, then property *Q* is shared by the sum of all QCSs exhibiting property *P*.
Table 1 summarizes the logical expressions proposed by Needham.

Table 1: the fundamental mereologic relationships

Identity of QCSs	$(x \subseteq y \wedge y \subseteq x) \rightarrow (x = y)$	(4)
Sum of all QCSs	$\exists x P(x) \rightarrow \exists! z\, (z = \sum y P(y))$	(5)
Distributive property	$(P(x) \wedge y \subseteq x) \rightarrow P(y)$	(6)
Cumulative property	$\exists x P(x) \wedge \forall x((P(x) \rightarrow Q(x)) \rightarrow Q(\sum x P(x))$	(7)

A formal definition of chemical substance

Now that we have clarified both the conventional definition of CS that we intend to adopt and the meaning of the fundamental mereological relationships, we may provide the formal definition of CS that will be the base of our subsequent argumentation.

[12] For a survey of the distinct formal techniques and the problems related with mereology, see (Champollion 2015; Harré and Llored 2011; Llored 2013; Llored and Harré 2014; Polkowski 2011; Varzi 2014).

[13] As far as the mereological aspects of our analysis are concerned, we have followed P. Needham (2012a). The flexibility of the mereological approach to the philosophy of chemistry has been well argued by Needham in several contributions, such (Needham 2013).

Let's designate with $\mathbb{A}$ the set of 129 million CSs indexed by the Chemical Abstracts Service (i.e. CSs provided with a CASRN) and with $\mathbb{T}$ the set of all known CSs, including those that are not to be registered for private interests, those that are going to be registered, those that are kept secret by national States, those illegal and those still unknown by the Control Authorities; then it is $\mathbb{A} \subset \mathbb{T}$, a condition indicating that $\mathbb{A}$ is an 'official' subset of all known CSs. Now, we define P_t as the property of *belonging to set* $\mathbb{T}$ and P_c as the property of *belonging to set* $\mathbb{A}$, i.e. being designated by a CASRN. It follows that:

$$P_c(x) \leftrightarrow x \in \mathbb{A} \quad (8)$$

Due to the existence of z - i.e. the sum of all the scattered quantities of a CS expressed by (5), and the distributive property expressed by (6) - it follows that all the QCSs that share the property P_c and contribute to the sum z, belong to set $\mathbb{A}$.

In this way, we assume that if $P_c(x)$ is true, then x is a QCS that instantiates a CS in specific conditions. We are aware that this statement has relevant implications; nevertheless, we choose it as the basic thesis of the present work and we will argue about it in the following sections.

Table 2
Symbols and espressions of predicate logic

Symbols and espressions	Meaning
x, y	Variable in a discourse domain
a, b, x_i, y_i	Constant in a discourse domain
$\mathfrak{R}_1$, $\mathfrak{R}_2$	Spacetime regions
$\in$, $\notin$	Belonging, non-belonging to a set
$\mathbb{A}$; $\mathbb{T}$	Set of CSs indexed by CAS; set of all CSs
$\mathbb{P}$	Set of properties
$\wedge$	Logical conjunction
$\vee$	Logical disjunction
$\rightarrow$	Material implication
$\leftrightarrow$	Double implication
$\exists$	Existential quantifier: there is al least an element such that …
$\nexists$	Existential quantifier: there is no element such that …
$\forall$	Universal quantified: all elements are such that ….
$\exists!$	Unicity existential quantifier: there is exactly one element such that …
$\neg$	Negation
ι	Definite description operator
P(x)	x exhibits property (expressed by) P
P(x,y)	x and y are related by property (expressed by) P
$\exists x P(x)$	There is at least one x such that P(x) is true

∀x*P*(x)	*P*(x) is true for all x
∃!x*P*(x)	There is exactly one x such that *P*(x) is true
ιx*P*(x)	x is the one/unique x such that

Chemical substances and spacetime regions: the insight offered by locative logic

Aim of the present research is the investigation of the changes undergone by the ontological status of a CS instantiated in QCSs found in very different contexts (research, production, commercialization and disposal). Different logic forms provide distinct strategies for describing the status of a QCS in each specific context. We might have adopted a temporal, diachronic logic that considers a QCS x at different times. The temporal aspect of CSs is clearly found in Quine: "We need all sorts of parts or portions of substances. For lack of a definable stopping place, the natural course at this point is to admit as an object *the material content of any portion of space-time*, however irregular and discontinuous and heterogeneous" (Quine 1981). Quine further specifies: "Milk, or wood, or sugar, is the discontinuous four-dimensional physical object comprising all world's milk, or wood, or sugar, ever" (Quine 1981). As our perspective insists on the presence of QCSs in distinct places, it seemed essential to use a logical form fit to account for the localization of the objects under study. We found useful Kris McDaniel's suggestions as regards the relation between mereology and localization (McDaniel 2014). Hence, we take his reference to *spacetime regions* (designed as $\mathfrak{R}_1$, $\mathfrak{R}_2$, etc.) as fundamental. The spacetime regions we deal with may be physical places, such as a chemical lab, an industrial plant or even an infrared spectrometer, or metaphorical places, such as the market.[14] In spite of our synchronic choice, we are well aware that the presence of a same CS in different places implies that such substance is stable enough to allow the transition from place to place. We take that aspect for granted and rather insist on the fact that, by laying in distinct locations, the QCSs can express distinct properties. In fact, a QCS *instantiates-at-*$\mathfrak{R}$ a property *P*: the relation of instantiation that links an object to a property, or some objects to a relation is always relative to a region. With Gilmore (2014), we remark that the sentence "an object O instantiates-at-$\mathfrak{R}$ a property *P*" describes the instantiation as a three-place relation between the object O, the property P and the region $\mathfrak{R}$; we formalize such relationship through the expression *Inst* ($\mathfrak{R}$, *P*, O). Based on the three mentioned elements, i.e. spacetime regions $\mathfrak{R}$, properties *P* instantiated-at-$\mathfrak{R}$, and QCS x, we may investigate the broad generality of the properties of a QCS x ∈ 𝔸, and discriminate four sets of properties, that we designate as $\mathbb{P}_1$, $\mathbb{P}_2$, $\mathbb{P}_3$, $\mathbb{P}_4$. Four possible cases have been spotted:

- ∀$\mathfrak{R}$∀x *Inst* ($\mathfrak{R}$, *P*, x) (that is: for any $\mathfrak{R}$ and any x, x instantiates property P in region $\mathfrak{R}$) is true if *P* is instantiated by *all* QCSs x in *all regions* $\mathfrak{R}$. If so, then *P* ∈ $\mathbb{P}_1$:

$$\forall\mathfrak{R}\forall x\ \textit{Inst}\ (\mathfrak{R}, P, x) \leftrightarrow (P \in \mathbb{P}_1) \qquad (9)$$

  - The most general example of *P* ∈ $\mathbb{P}_1$ is the simple occupation of a part of region $\mathfrak{R}$ by QCS x.
  - *P* ∈ $\mathbb{P}_1$ may be 'to have mass'; 'to have chemical composition'; 'to absorb or to emit electromagnetic radiation'; P_c or 'to have a CASRN'. From the ontologic viewpoint, the above-listed properties are strongly different: 'to have mass' is a macroscopic property of the QCS; the ability 'to absorb or to emit electromagnetic radiation' is a microscopic property; 'to have a CASRN' has a conventional character.
  - As for the instantiation of these properties, the role played by the region may be limited to the hospitality offered to the QCS. In fact, it is often the observer that -

[14] Whatever $\mathfrak{R}$ can be, complying with Quine, when region $\mathfrak{R}$ becomes a variable bound by an existential operator, an ontological committment is taken towards it.

based on its theoretical and circumstantial knowledge – assign x a certain property *P* in different situations. Let's take, for example, the property of having a chemical composition P_{comp}: by reading the label on a can $\mathfrak{R}$, the observer is persuaded that the content x is such that ιx *Inst* ($\mathfrak{R}$, P_{comp}, x); the expression reads "this very QCS x instantiates the composition P_{comp} in can $\mathfrak{R}$".

- The broad generality of $P \in \mathbb{P}_1$ recalls the fundamental thermodynamic properties: *P* may be enthalpy, entropy, chemical potential. Note that these properties can be defined for any x in any $\mathfrak{R}$; nevertheless, we can quantify *P* only if $\mathfrak{R}$ is a closed system and x is in thermodynamic equilibrium with $\mathfrak{R}$.

- $\exists\mathfrak{R}\forall$x *Inst* ($\mathfrak{R}$, *P*, x) (that is: for any x there is at least one region $\mathfrak{R}$ wherein x instantiates property *P*) is true if *P* is instantiated by *all* QCSs x in *at least* one region $\mathfrak{R}$. If so, then $P \in \mathbb{P}_2$:

$$\exists\mathfrak{R}\forall x\ Inst\ (\mathfrak{R}, P, x) \leftrightarrow (P \in \mathbb{P}_2) \qquad (10)$$

  - If $\mathfrak{R}$ is a mass spectrometer (conveniently equipped) and *P* is a mass spectrum, all QCSs x (conveniently prepared) may instantiate *P* in $\mathfrak{R}$. It is possible to go into further details as the QCS x is found in a holder $\mathfrak{R}_1$ that is part of chamber $\mathfrak{R}_2$ of an instrument $\mathfrak{R}_3$ located in room $\mathfrak{R}_4$ of a laboratory $\mathfrak{R}_5$. We will recur to a synecdoche, by referring to the chemical-physical lab instead of specifying its sub-regions. The reader may well imagine the sub-regions a QCS may be related with.
  - $P \in \mathbb{P}_2$ may be "to provide a spectrum_____", to be completed according to the any kind of spectroscopy (IR emission, Uv-Vis, etc.).
  - If we focus on physical states (solid, liquid or gaseous), only 'to be solid' is a property $P \in \mathbb{P}_2$ because many CSs decompose before melting: the property 'to be solid' depends on temperature; hence it depends on $\mathfrak{R}$ and cannot be generalized to whatever $\mathfrak{R}$. Therefore, as all properties depending on $\mathfrak{R}$, 'to be solid' is a relational property.
  - The standard enthalphy of formation of a CS is a further example of property associable to whatever CS, albeit only in a specific region $\mathfrak{R}$. In this case, $\mathfrak{R}$ has a virtual and specific character because it corresponds to the conventionally defined 'standard conditions'. The tables that list values of standard thermodynamic quantities are virtually valid for any x, but they refer exclusively to the 'standard' region $\mathfrak{R}_{st}$.
  - The stability *P* of a CS is essential for defining the CS as such: in order to detect (and even more strictly, to identify and characterize) whatever CS, there must be at least a region $\mathfrak{R}$ wherein the CS remains unchanged over a definite (albeit short) time interval. Despite its stringent character, this *P* is not an intrinsic property: it is rather relational; in fact, stability is strictly dependent on specific temperature and pressure conditions, as well as on the absence of other CSs that might react with the CS under investigation and chemically transform it.

- $\forall\mathfrak{R}\exists$x *Inst* ($\mathfrak{R}$, *P*, x) (that is 'there is al least one x that instantiates property *P* in all regions $\mathfrak{R}$') is true if *P* is expressed by *at least* one QCS x in *all regions* $\mathfrak{R}$. If so, then $P \in \mathbb{P}_3$:

$$\forall\mathfrak{R}\exists x\ Inst\ (\mathfrak{R}, P, x) \leftrightarrow (P \in \mathbb{P}_3) \qquad (11)$$

  - The properties $P \in \mathbb{P}_3$ are clearly discriminant as compared to properties $P \in \mathbb{P}_1$. A relevant case concerns radioactive CSs that keep radioactive in whatever region and consequently have, for example, an intrinsic half-life. Similar cases are that of polar CSs (which exhibits a permanent dipole moment that is independent from the *spacetime* region $\mathfrak{R}$), or of CSs made of atoms or molecules with an odd number of electrons.

- Properties $P \in \mathbb{P}_3$ are intrinsic of CSs, i.e. independent from the *spacetime* region $\mathfrak{R}$, although $\mathfrak{R}$ may exert a modulatory action. This is the case of CSs with a specific functional group that confers a CS a specific reactivity. The recognition assays typical of organic chemistry are grounded on this property. Region $\mathfrak{R}$ may modulate the kinetic or the thermodynamic of a process, but it does not influence the ability of these of CSs to react in a specific way that is related with the functional group owned by the molecule.

- $\exists\mathfrak{R}\exists x$ *Inst* ($\mathfrak{R}$, *P*, x) (that is 'there is at least one x that instantiates property *P* in at least one region $\mathfrak{R}$') is true if *P* is expressed by *at least* one of QCSs x in *at least* one region $\mathfrak{R}$. If so, then $P \in \mathbb{P}_4$:

$$\exists\mathfrak{R}\exists x \; Inst\ (\mathfrak{R}, P, x) \leftrightarrow (P \in \mathbb{P}_4) \qquad (12)$$

  - In this case, the relationship between QCS and region wherein property *P* is instantiated becomes very selective. This is the most interesting situation for a chemist; we will provide a few examples. $\mathfrak{R}$ may be a tumor cell and x may be a QCS that may instantiate the death of such cell (e.g. a monoclonal antibody that selectively recognizes a receptor found only in that specific kind of cell), leaving the others undamaged. $\mathfrak{R}$ may be a solution containing ketons and aldehydes and x may be a reactant that instantiates the separation of aldehyde and ketones.[15]
  - Some properties that belong to this class may be designated as macroscopic in that they are expressed only beyond a certain level of aggregation (e.g. malleability, electric conductivity, etc.).[16]
  - All toxicity and ecotoxicity properties are $P \in \mathbb{P}_4$. In these case $\mathfrak{R}$ may be a natural or an artificial environment, a 'model organism', etc. If *P* is the property 'to be toxic', then expression $\exists\mathfrak{R}\exists x$ *Inst* ($\mathfrak{R}$, *P*, x) explicitly highlights that the toxicity depends on the region $\mathfrak{R}$ where the QCS x is found.
  - Properties belonging to this group are specific of a CS but they have also a relational character. For example, capillarity is a property that may be instantiated by a specific QCS in a specific region $\mathfrak{R}$ as it depends very strictly on intermolecular interactions between the investigated CS and the material which the capillar walls are made of. In other words, such property – referred to a specific QCS x – may be instantiated only if region $\mathfrak{R}$ exhibits specific features. This is a classic example of a situation where spatiality (intended as relationship between QCS and region $\mathfrak{R}$) plays a crucial role.
  - Even structural properties typical of supramolecular systems belong to this set, precisely due to their relational character: e.g. the possession of a specific tertiary structure by a given protein. Tertiary structure is typical of a protein and depends strongly on region $\mathfrak{R}$. When boundary conditions change, tertiary structure may fail: hence this is not an intrinsic property despite its being a structural property.

Table 3 summarises the classification of the properties of CSs in relation to both the CS and the regions wherein these properties are instantiated.

Table 3: Formal definition of the 4 sets of properties

Definition	Features of *P*	
$\forall\mathfrak{R}\forall x$ *Inst* ($\mathfrak{R}$, *P*, x) $\leftrightarrow$ ($P \in \mathbb{P}_1$)	$P \in \mathbb{P}_1$ is intrinsic and general; e.g. to have mass	(9)

[15] This is the case of the 'Girard and Sandulescu' reactant, patented in 1936; this reactant had a fundamental role in the chase of cortison (Cerruti 1998).

[16] In the present investigation – already quite extensive – we neglect the problem of CS' or system's phases. On the philosophical problems related with phases see (van Brakel 1986; Needham 2012a and b; Vemulapalli 2012).

$\exists\mathfrak{R}\forall x\ Inst\ (\mathfrak{R}, P, x) \leftrightarrow (P \in \mathbb{P}_2)$	$P \in \mathbb{P}_2$ is extrinsic and general; e.g. to exhibit a mass spectrum	(10)
$\forall\mathfrak{R}\exists x\ Inst\ (\mathfrak{R}, P, x) \leftrightarrow (P \in \mathbb{P}_3)$	$P \in \mathbb{P}_3$ is intrinsic and specific, e.g. to be radioactive	(11)
$\exists\mathfrak{R}\exists x\ Inst\ (\mathfrak{R}, P, x) \leftrightarrow (P \in \mathbb{P}_4)$	$P \in \mathbb{P}_4$ is extrinsic and specific, e.g. to be toxic towards the environment	(12)

In a region $\mathfrak{R}$ many different activities may take place, by human beings, devices, machineries, plants, signs; the region enables the object to instantiate a specific property by entailing an *active* relationship with it; in other words, a property is implemented in a region $\mathfrak{R}$ through peculiar *regional activities*. On the other hand, a specific and fundamental 'activity' fulfilled by the spacetime region is the actual ospitality of the object.

In the following sections we will need to specify the $\mathfrak{R}_i$ that is treated at each time; once $\mathfrak{R}_i$ is defined, the four relationships of Table 3 reduce to two cases. In the first case:

$$\forall x\ Inst\ (\mathfrak{R}_i, P, x) \rightarrow ((P \in \mathbb{P}_1) \vee (P \in \mathbb{P}_2)) \quad (13)$$

In this case, properties P are general and may be either intrinsic ($P \in \mathbb{P}_1$) or extrinsic ($P \in \mathbb{P}_2$), that is dependent on $\mathfrak{R}_i$. In the other case:

$$\exists x\ Inst\ (\mathfrak{R}_i, P, x) \rightarrow ((P \in \mathbb{P}_3) \vee (P \in \mathbb{P}_4)) \quad (14)$$

In this case, properties P are specific and may be intrinsic ($P \in \mathbb{P}_3$) or extrinsic ($P \in \mathbb{P}_4$).

Notation *Inst* ($\mathfrak{R}$, P, x) is effective by putting $\mathfrak{R}$ as argument of *Inst*. Nevertheless, when the instatiation relation *Inst* ($\mathfrak{R}$, P, x) is referred to a preset region $\mathfrak{R}_i$, the heavy triadic notation can be simplified, as the presence of $\mathfrak{R}$ amongst the arguments of *Inst* becomes redundant. This becomes clear by comparing the two sentences:

(i) "x *istantiates-in-*$\mathfrak{R}_i$ the property P" and (ii) "x *has* the property P"

If $P \in \mathbb{P}_1$, it is intrinsic to the QCS x: for example, P is "to have mass". Then (i) may be rewritten as (ii):

"x *istantiates-in-*$\mathfrak{R}_i$ the property "to have mass" = "x *has* mass"

In addition, this P is instantiated by any x in any $\mathfrak{R}$**.** In this case, the instantiation activity is reduced to pure locative ospitality offered by $\mathfrak{R}_i$ to x; hence, for $P \in \mathbb{P}_1$ we may definitely write P(x). If $P \in \mathbb{P}_3$ not all QCSs x are such that P(x), and the monadic relation is true only if "x has/is P".[17]

The instantiation of extrinsic properties $P \in \mathbb{P}_2$ e $P \in \mathbb{P}_4$ depends on the location of x in one or more regions. In these cases, a *relational activity* between $\mathfrak{R}$ and x is required in order for these properties to be expressed by the QCS. A couple of examples will clarify the relational distinction between intrinsic and extrinsic relation.

If P_{mass} = "to have mass", then we state that $P_{mass} \in \mathbb{P}_1$; if $P_{mspectr}$ = "to have a mass spectrum" then we state that $P_{mspectr} \in \mathbb{P}_2$. A QCS x has a mass wherever it is; hence P_{mass}(x) is true in all regions. A QCS x has a mass spectrum only when it interacts with a mass spectrometer. Hence, by writing $P_{mspectr}$ (x) we intend that "x (in the proper conditions) provides a mass spectrum". The last class of properties to be considered is $P \in \mathbb{P}_4$. We have already underlined the selectivity of these properties. In fact, in this case, the relational activity between QCS and region is strict: this is the case of the relation described by the *Schlüssel-Schloss-Prinzip* proposed by Emil Fischer in 1894 (Fischer 1894). For $P \in \mathbb{P}_4$ the presence of the region cannot be tacit: we will treat these properties as dyadic relations.

[17] The grammar form depends on the natural language in use and on the specific property P.

The logical apparatus at work

In the previous sections we have shown and commented the analytical apparatus that we intend to apply for arguing about the ontological status of a CS synchronically instantiated in distinct locations:

Chemical substance ⇨ material ⇨ (industrial) product ⇨ goods ⇨ waste

More in details: i) we have discussed the possibility of using locative logic for spotting the properties of a given CS instantiated in QCSs placed in distinct spacetime regions; ii) we showed that this treatment may find a formal expression through a regimentation process based on first-order predicate logic; iii) we showed that mereologic logic, that helps defining the relationship between CS and QCSs, is compatible with such treatment; iv) we identified 4 sets of properties of CSs, based on their intrinsic/extrinsic and/or general/specific character. In the following sections we will apply this logical apparatus to the analysis of the status of a CS instantiated in the aforementioned locations, from an ontological standpoint.

Implications of being a chemical substance in a chemical lab

In the lifecycle of a QCS, the 'chemical lab' is certainly the starting point as it is the place where the QCS is characterised and identified as instantiation of a specific CS. The QCS may be synthesized or isolated from a natural source: no matter what its origin is - and taken for granted that we deal with known CSs - the problem of its identification remains: one has to check if the (synthesized or isolated) QCS is actually the instantiation of the desired CS; hence, the importance of identification. The 'chemistry lab' is an ideal spacetime region, designed as $\mathfrak{R}_{\mathbf{CL}}$, whose scientific staff and instrumental equipment are suitable for a QCS x to express property *P*, thus making the expression *Inst* ($\mathfrak{R}_{\mathbf{CL}}$, *P*, x) true. We choose to consider only $x \in \mathbb{A}$; hence we write:

$$\forall x \; Inst\,(\mathfrak{R}_{\mathbf{CL}}, P_c, x) \rightarrow P_c(x) \qquad (15)$$

Expression (15) refers to known QCSs ($x \in \mathbb{A}$). If $\mathfrak{R}_{\mathbf{CL}}$ was a lab where syntheses of new CSs are performed, it would be $\exists x(\neg\, Inst\,(\mathfrak{R}_{\mathbf{CL}}, P_c, x))$. Let's go back to the 4 sets of properties listed in Table 3.

The first set ($P \in \mathbb{P}_1$) includes fully general properties, to the point that these are not much informative with respect to the problem of identifying the CS. Their importance comes from their being intrinsic properties, as they are the necessary premises for introducing the other sets of properties. This category includes 'to have mass', 'to have chemical composition', 'to absorb and to emit electromagnetic radiation', or to exhibit some specific thermodynamic properties. These last, in particular, are important for the definition of chemical potentials or aggregation states.

The second set, $P \in \mathbb{P}_2$, shifts from intrinsic to extrinsic properties, whose instantiation implies an active role of the concerned region. We have already underlined that these are relational properties, as they can be defined only by relating each QCS x with a specific region $\mathfrak{R}$. This is the case of standard enthalpies and entropies of formation that refers to the virtual region identified by the conventional standard conditions. Hence, the role of region $\mathfrak{R}$ is critical for this set of properties, as when $\mathfrak{R}$ is changed the property is no longer expressed or expressible. This clarifies the crucial difference between properties *P* belonging to $\mathbb{P}_1$ and $\mathbb{P}_2$, respectively. While 'to have mass' is independent from region $\mathfrak{R}$, the instantiation of a mass spectrum is impossible outside the region represented by the mass spectrometer.

With the third set of properties, i.e. $P \in \mathbb{P}_3$, we get back to intrinsic features of CSs. These properties are independent from the region, but specific for a given CS; hence they are useful for its identification. Radioactivity and polarity are good representatives of this set of properties, as both inherently depend on the physical constitution of the CS, and not on its interactions with the environment. Another property belonging to this set is the possession of a specific functional group: most part of the synthetic activity is aimed at introducing specific functional groups in specific

positions of a molecule, in order to provide it with a precise chemical reactivity or the possibility of interacting specifically with a target. In general, category $P \in \mathbb{P}_3$ may include structural properties although not any structural property is independent from the region. For example, proteins exhibit tertiary and quaternary structures that are partly determined by the chemical environment.

This leads us to the fourth set of properties, $P \in \mathbb{P}_4$, dependent on both the region and the kind of CS. These have an extrinsic and specific character. The relational character of this class of properties finds here a further specification, and becomes binary. This is the case of solubility, that is specific of each CS in relation with each specific solvent: $P_{sol}(x,y)$ means that the QCS x is soluble in the QCS y. Binary relationships are fundamental for characterising the relation of CSs belonging to set $\mathbb{A}$. The notation that we have adopted allows describing the behaviour of CSs with respect to various solvents. For example, would the expression

$$\forall x P_{sol}(x,x_i) \tag{16}$$

be true, we would have found in x_i the mythical universal solvent. Conversely, chemists hope this expression to be true:

$$\forall x \exists y P_{sol}(x,y) \tag{17}$$

It means that for any CS there is at least one solvent; unfortunately, it is often true that $\nexists y P_{sol}(x_i,y)$: QCS x_i is insoluble in all known solvents.

Materials

In order to define a 'material' in our context, we will refer to the knowledge shared by the community of material scientists. The *Journal of Materials Science*, an important journal of that disciplinary field, lists different kinds of materials: "metals, ceramics, glasses, polymers, electrical materials, composite materials, fibers, nanostructured materials, nanocomposites, and biological and biomedical materials" (Springer 2015). Once again, the list highlights the heterogeneous criteria adopted for the classification, e.g. the undifferentiated reference to intrinsic and extrinsic properties. In addition, the items are not mutually exclusive: e.g. an electric material may also be nanostructured. The journal *Nature Materials* presents itself as follows: it "covers all applied and fundamental aspects of the synthesis/*processing*, structure/composition, properties and *performance* of materials, where 'materials' are identified as substances in the condensed states (liquid, solid, colloidal) designed or manipulated for technological ends" (Nature 2015). The broad variety of materials makes difficult to spot properties shared by all of them, useful to define them; nevertheless, we sought for selection criteria taking the risk of neglecting some typologies. Since several decades, it has been stated that in order to have a material, specific *performances* must be achieved by *processing* a given quantity of matter. This commitment is confirmed by Ohring in the introduction of his book: "the tetrahedron of *processing*-structure-properties-*performanc*e interactions, the multi-faceted *processing*-structure concerns are the ones this book primarily focuses on" (Ohring et al., 2014, p. xiv). According to standard definitions, *materials processing* indicates the series of operations that transforms industrial materials from a raw-material state into finished parts or products (Encyclopædia Britannica 2015). The possibility to material processing a QCS is a premise for its employability as material; nevertheless, most part of material research is rather addressed towards the improvement or the appearance of (new) performances. An important case is represented by nanomaterials research, as these are a strongly innovative set of materials. We will recall it further on.

Based on the previous specifications, we will designate as P_{proc} the property of *being processed*, and with P_{perf} the property of *showing a performance*. In the applicative context, expression $P_{proc}(x) \wedge P_{perf}(x)$ has to be interpreted in its logical value: the fact that the QCS x is processed is not sufficient; the QCS must also exhibit some relevant performance (e.g. 'impermeability', 'resistance to traction', 'to be a reference material', etc.). We designate as P_{ma} the

property of *being a material*. Expression $P_c(x) \wedge P_{proc}(x) \wedge P_{perf}(x)$ is true whenever a QCS x is provided with a CASRN (i.e. it belongs to set $\mathbb{A}$), it is processable and exhibits a performance; in this case we state that $P_{ma}(x)$ is true:

$$\forall x((P_c(x) \wedge P_{proc}(x) \wedge P_{perf}(x)) \rightarrow P_{ma}(x)) \quad (18)$$

[QCSs belonging to set $\mathbb{A}$, processable and capable of a performance are materials]

The meaning of (18) is clarified by an example: the QCS x is synthesized in a powder form; it must undergo a processing phase in order to become a material (e.g. it has to be melted and extruded as a fiber) and to exhibit a certain resistance to traction (plus a number of other performances). A relevant aspect of materials is that their properties can be modulated according to the necessity.
Another example is represented by thermoplastic polymers, whose transition to materials may be followed by taking as a reference quantity the Melt Flow Index (MFI). MFI is a measure of the ease of flow of the melt of a thermoplastic polymer. It is defined as the mass of polymer, in grams, flowing in ten minutes through a capillary of a specific diameter and length by a pressure applied via prescribed alternative gravimetric weights for alternative prescribed temperatures. Melt flow rate is very commonly used for polyolefins, polyethylene being measured at 190°C and polypropylene at 230°C. The plastics engineer should choose a material with a melt index high enough that the molten polymer can be easily formed into the article intended, but low enough that the mechanical strength of the final article will be sufficient for its use. MFI is a clear example of properties $P \in \mathbb{P}_4$ as it is both region- and material-dependent.
Many CSs are prepared and purified in a specific way, their compositions and properties are verified in order to use these CSs as *reference material* in various lab practices. World Health Organisation provides this definition: “The term *chemical reference substance* […] refers to an authenticated, uniform *material* that is intended for use in specified chemical and physical tests, in which its properties are compared with those of the product under examination, and which possesses a degree of purity adequate for its intended use” (WHO Expert Committee on Specifications for Pharmaceutical Preparations 2007). A QCS of a common CS such as Lead(II) nitrate, conveniently processed, becomes - in the current practice - a material finalized to clear-cut aims, described in these terms: “primary reference material (for complexometry), certified standard titrimetric substance” (Sigma Aldrich 2015). In these cases P_{proc} corresponds to the process of preparation of the QCS to become a standard material: its P_{perf} is instantiated, for example, in the calibration of an analyitical instrument.

A further class of materials that deserves attention is represented by nanomaterials, considering the singularity of the CS-material relationship that they represent. The European Union legal definition is the following: "‘Nanomaterial’ means a natural, incidental or manufactured material containing particles, [...] where, for 50 % or more of the particles in the number size distribution, one or more external dimensions is in the size range 1 nm-100 nm". Immediately after this specification, some exceptions are introduced: “fullerenes, graphene flakes and single wall carbon nanotubes with one or more external dimensions below 1 nm should be considered as nano-materials”. Finally, the European document underlines a difficult aspect: “Measuring size and size distributions in nanomaterials is challenging in many cases and different measurement methods may not provide comparable results” (EU Commission 2011).[18] The fact that nanomaterials may be “a natural, incidental or manufactured material” levels nature, fate and industry. Hence, according

[18] We have chosen to mention the EU definition because, at present, it is the only one with a legal value. Nevertheless, other definitions by Public Authorities are available: an interesting analysis of the various, sometimes contradictory definitions of nanomaterials, was published on November 2014 by three non-governmental organizations: Center for International Environmental Law, European Citizen’s Organization for Standardization, Öko-Institut, “Nanomaterials Definition fact sheet”, available at URL: http://www.ciel.org/Publications/Nano_definition_Nov2014.pdf

to the European legislator, in nature and/or by chance, expression (18) is redundant and the simpler $\exists x(P_{ma}(x))$ is true: the man's role is cancelled.

The case of industrial catalysts is interesting from both the ontologic and cognitive viewpoints. The current disciplinary language is ambiguous as whether the catalyst is to be intended as a CS or a material. In the starting chapter of an important textbook on heterogeneous catalysis we find that "a catalyst is a material that converts reactants into products through a series of elementary steps", and the authors add that "Another definition is that a catalyst is a substance that transforms reactants into products, through an uninterrupted and repeated cycle of elementary steps". Clearly, the authors do not raise any doubt on such ambiguity; nevertheless, they adopt these descriptive terms immediately after: "a solid material", "a high-surface area material" (Dumesic et al. 2008, p.1).[19] In general, in the industrial context, the system that is introduced into the reactor is a mixture of distinct CSs (catalysts, co-catalysts, supports, etc.), and the real (practical) value of a catalyst depends on a number of parameters (selectivity, yield, lifespan, etc.). Some of them depend directly on the CS that actually speeds up the reaction(s), whereas other results exclusively or cooperatively from the CSs found in the reactor. The alternative between CS and 'material' is neither a semantic exercise not an ontological judgement because chemists, depending on their disciplinary label, exploit distinct theoretical models. Experimentalists treats catalytic systems as complex systems (i.e. materials), and they employ *ad hoc* sets of rules and 'local' theories that help them in driving lab practices, choosing a reactor model, assessing the kinetic and thermodynamic parameters. Theoretical chemists have the tendence to study the catalytic activity *stricto sensu* of surface active sites through quantum and statistical mechanics models. Nevertheless, the success of a catalyst is the result of a tremendous knowledge effort, fed by an information and knowledge flow coming from production plants. If that productive success makes a material ontologically an industrial catalyst, then we have to assign the same epistemic value to any single bit of knowledge or of practical action which contributes in a necessary way to the final success (Cerruti 1999).

It is worth remarking that expression (18) includes also non traditional materials, such as medicinal drugs, that may be seen as materials that cannot be processed or - as an alternative – materials whose formulation can be seen as an expression of their 'processability' in a wide sense. For example, slow-release drugs are usually based on formulations that exploit inclusion complexes where, for example, the active principle is trapped into a cyclodextrin. Similarly, the control of pharmacodynamics or of the drug's absorption in specific districts of the organism, or still the need for protecting the active principle from chemical degradation due to endogen CSs, require the principle to be included in liposomes. Several variants are possible and they correspond to distinct formulations of an active principle that could not be effectively administrated as such.[20] A somehow similar case is provided by detergents, either fluid or solid, for which the problem of formulation is important as well.

Products

Remember that TIME is Money.
Benjamin Franklin (1748)

In our context, we designate as 'product' the final outcome of an industrial process, obtained in a timelength and amount sufficient to distinguish it from the lab product. We underline the reference to time: clearly, this does not mean that a chemical lab does not pay attention to time but, for the industrial production, time assumes the connotation highlighted by Franklin: time is money. 'Plant capacity' means the maximum quantity of product that can be produced by time unit in the plant

[19] Further on in the text, catalysts are characterized through their *performance*: "The central level of research and development of heterogeneous catalysts involves the quantification of catalyst performance" on p.10.

[20] More than 40% of new chemical entities developed in pharmaceutical industry are practically insoluble in water (Savjani et al. 2012).

with the existing equipment. The nominal capacity of a plant is assessed in tons/year, and the 'economies of scale', so important for chemical industry aim at increasing the capacity to huge values.

A property that discriminates a product from CSs or materials produced in the lab is its production cost. We designate with P_{pc} the property *to have a production cost* whereas P_p is the property of *being a product.* It is then possible to write:

$$\forall x\ ((P_{ma}(x) \wedge P_{pc}(x)) \rightarrow P_P(x)) \quad (19)$$

[materials with a production cost are products]

$$\forall x((P_c(x) \wedge P_{proc}(x) \wedge P_{perf}(x) \wedge P_{pc}(x)) \rightarrow P_P(x)) \quad (20)$$

[QCSs belonging to set $\mathbb{A}$, processed, with a performance and a production cost are products]

The following expression is also true:

$$\forall x((P_c(x) \wedge P_{pc}(x)) \rightarrow P_P(x)) \quad (21)$$

It refers to QCSs that become products without being materials, as they lack the typical properties of materials but they exhibit those of products (e.g. ammonium nitrate employed as fertilizer, ethylene, etc.). A more in-depth discussion of expression (21) is beyond the scopes of the present research. We just would like to mention that some CSs becomes 'products' (in huge amounts), without necessarily exhibiting peculiar performances, apart from their physical-chemical inhenerent ones, such as reactivity or solvent ability. In important chemical industries, such as the pharmaceutical or the detergent ones, the following expression is valid:

$$\forall x((P_c(x) \wedge P_{perf}(x) \wedge P_{pc}(x)) \rightarrow P_P(x)) \quad (22)$$

The performances recalled by expression (22) are the physiological ones (for drugs) or the tensioactivity and the detergence power (for detergents).

An essential difference between a material and a product deals with the different 'openness' of the *information* about the material or the product. The material science lab tends to continuously change the pool of information concerning a given material, by improving its performances or seeking for new applications: the information on the material is open. In an industrial plant, information on the material to be produced defines a rigid protocol that has to be followed strictly: information on the material is closed, whereas the knowledge that allows a better and better fulfillment of the protocol within the plant is open. This aspect includes the role played by human experience in keeping the plant at its best performances, by adjusting continuously the operating conditions, if needed.

On the market

We call 'goods' those products or QCSs that are put on sale on the market. We refer to the legal market, regulated by stringent rules and laws. A preliminary property of the product is 'to be compliant with legal standards' (i.e. to comply with current REACH rules, etc.). We designate with P_{cpl} the property to *be compliant*. The second crucial feature of the product is its being purchasable: the product must have a price, transactions must be taxed, the product must actually enter the market. We designate as P_{pur} the property of *being purchaseable* and as P_{go} the property of *being goods*:

$$\forall x((P_P(x) \wedge P_{cpl}(x) \wedge P_{pur}(x)) \rightarrow P_{go}(x)) \quad (23)$$

[products compliant with the rules and purchasable are goods]

$$\forall x((P_c(x) \wedge P_{proc}(x) \wedge P_{perf}(x) \wedge P_{pc}(x) \wedge P_{cpl}(x) \wedge P_{pur}(x)) \rightarrow P_{go}(x)) \quad (24)$$

[QCSs belonging to set $\mathbb{A}$, processed, exhibiting a performance, with a production cost, compliant with the rules and purchaseable are goods]

It is worth underlining that whenever a QCS is part of goods, the region 'market' enriches the ontology of the object-goods because this kind of objects is involved in a wide net of relationships. Some relationships fall within the area of economic and social sciences, e.g. when the goods undergo marketing surveys, lifecycle assessments, investigations on status symbols, etc. Others relationships concern marketing techniques, from advertisements to promotional and expositive techniques. These are counterbalanced by the attention of consumers'associations, authorities' surveillance (adverts trustiness, possible toxicity, etc.) and private citizens' surveillance (legal protection of patents and brands). Finally, one has to consider the goods-purchaser relationships, quite varied and imponderable. In our society, the property of being goods $P_{go}(x)$ seems to be the highest possible 'ontological achievement' of a CS.
From a diachronic viewpoint, whenever a good is acquired, an ownership change occurs. This change is important as the transition from CS to material and goods might occur without any change of ownership. But a sale implies unavoidably such a change. This fact acquires some relevance with respect to the problem of wastes.

Waste and its problematic fate

Goods may become waste in a number of different ways. Here are some examples: unsold goods due to obsolescence; unsold goods due to their not being competitive as compared to other goods; goods that cannot be sold because are damaged; goods that have been sold, employed and that subsequently became (or were judged) no longer employable. In all four examples, waste has a common property, e.g. a 'negative price' or rather a cost related with its disposal. Let's designate as P_{dc} the property to *have a disposal cost* and as P_{disp} the property of *being disposed of*. By designating as P_{lw} the property of *being a legal waste*, we can write:

$$\forall x((P_c(x) \wedge P_{dc}(x) \wedge P_{disp}(x)) \rightarrow P_{lw}(x)) \qquad (25)$$

[QCSs belonging to set $\mathbb{A}$, with a disposal cost, and that have been disposed of, are legal waste]

Clearly a QCS may become waste at any step between the chemical lab and the market. As a legal waste, a QCS loses a number of relationships but it maintains its chemical composition as a known property. This property is essential in defining its practical and economic fate. The QCS regresses to a looser classification, but not all information about it is lost. It has to be said that, would expression (25) always apply to the real world, pollution would be more restrained. Unfortunately, expression (25) sometimes simplifies dramatically into:

$$\exists x(P_{disp}(x) \rightarrow P_{iw}(x)) \qquad (26)$$

[a QCS that has been (only) disposed of is an illegal waste]

This is the case when a QCS x becomes an *illegal waste* $P_{iw}(x)$. Whenever a waste is dropped out in the environment, a dramatic loss of information occurs because its very same chemical identity is lost or neglected. This is the reason why the basic property $P_c(x)$ is no longer included in expression (26).
A further crucial difference between legal and illegal waste concerns their ownership. The legal transition from goods to waste implies a change of ownership, but the owner can still be identified. Conversely, an illegal waste has no longer an owner. Hence, whereas a legal waste is part of a socio-economic virtuous cyle, an illegal waste represents a dead endpoint.
The ontological status of waste has not attracted much attention by the philosophers of chemistry, in spite of the social relevance of the waste issue and the related negative place occupied by chemistry in the collective imagination. Nevertheless, there is a more general reflection on wastes and some results are relevant to the chemical context. Jane Bennett, through a phenomenological approach, underlined the 'power loss' undergone by the material object, either made up by men or natural, when it becomes a waste: "Trash, garbage, litter, dirt, debris, filth, refuse, detritus, rubbish,

junk: materialities without their thing-power". Bennett presents her contribution as "a speculative onto-story", and in fact she refers to a relational ontology: "the agential powers of natural and artifactual things, [...] the dense web of their connections with each other and with human bodies" (Bennett 2004). With a different approach, Gay Hawkins investigated the multiple relationships involving wastes in our society, at the public or individual level. Overall, these relationships outline an ethos to which one complies without reflection; nevertheless – according to Hawkins – a different way is possible, by making oneself conscious of the "daily rituals of dealing with ourselves and our rubbish. […] The minute you start paying attention to waste a different relation with it is enacted [...] letting it confront us not as worthless detritus but as provocative things that just might make us consider what we do" (Hawkins 2006, p.13). Jennifer Gabrys got to similar conclusions as Hawkins: she investigated in-depth the story and the problems related with "digital rubbish", and she stated that "waste is more than a heap of defunct objects; it is also a mixture of fickering and mutable relations. Through waste, it is possible to think a 'new object'" (Gabrys 2013, p. 149). These reflections highlight that the ontological-relational depletion that occurs when something shifts from object-of-current-use to waste, can to some extent be recovered through the establishment of new relations. This is exactly what - at the institutional and disciplinary level – do chemists that are experts of waste recycling and disposal. The philosophical aspects of CSs reduced to waste go beyond the immediate economical and ecological connotation. This is Kevin Taylor's position that calls for the need of an "ontological humility" by those who really seek for a solution of environmental problems (Taylor 2011).

A final glance to the whole landscape

The results of the regimentation process are summarised in Table 4. Before getting an overall final glance to the status of a CS instantiated in different locations, it is worth addressing an aspect that has been mentioned, but not analysed in the previous sections. We refer to the information and knowledge content that characterizes the various steps that have been examined. In each one of the examined situations, a QCS is equipped with *knowledge* and *information* acquired during the manipulations experienced on its way to the location. It seems relevant to spend few words for restating the distinct meaning of these two terms. Intuitively, one can say that there are different types of knowledge, e.g. acquaintance knowledge (I *know* London well), ability knowledge (I *know how* to cook a quiche lorraine), and propositional knowledge (I *know that* all crows are black). The distinction between 'know how' and 'know that' was introduced in 1945 by the English philosopher Gilbert Ryle.[21] *In nuce* 'knowing how' is a way of knowing that is based on experience and it is aimed at providing/getting performances; 'knowing that' is a way of knowing based on rules and operational procedures aimed at describing/explaining states of the world, properties, relations, processes. For example, it is clear that the researcher's ability is not grounded on the pure knowledge of laws, rules and operational procedures, albeit necessary; it is also grounded on its ability to adopt suitable strategies (stemming from experience), on its critical thinking, its intuition, its ability to understand the specificity of a context, etc. In the years that followed the publication of Ryle's work the distinction between 'know how' and 'know that' was discussed and criticised several times, expecially because a radical interpretation of Ryle's thought leads to the evident impossibility to reduce all the knowledge about a specific 'know how' to a correlate 'knowing that', that may be completely expressed by a natural language. One could say that *knowing how cannot be defined in terms of knowing that*. In other words, only '*know that'* (i.e. propositional knowledge or information) can be formalised by predicate logic, whereas '*know how'* cannot be fully codified. This also means that only '*know that'* may be the input of a computer or be the object of systematic classifications within informatic databases; in fact, transmission of a '*know how'* implies necessarily an interaction between human individuals.

[21] A deep analysis of the logical aspects and philosophical implication of this distinction may be found in the original text 'The Concept of Mind' published in 1949 (Ryle 1949).

Column 2 of Table 4 aims at highlighting where, in the different regions $\mathfrak{R}$, the information content intertwines with the knowledge content.
Column 3 of Table 4 reports the logical expressions that formalize the status of a QCS in distinct regions $\mathfrak{R}$, according to predicate logic. It seems important to underline that Table 4 relies only on relational properties that are dependent on the region $\mathfrak{R}$ where the QCS is found and may be inherited or lost by the QCS.
A glimpse to such expressions clearly shows that the status changes from region to region, as the number of predicates increases or decreases. According to Quine's lesson, the changes highlighted by the logical expressions are neither merely qualitative nor just intuitive: in fact, the regimentation procedure points out the ontological commitments that are implicit in the formal language. The Table shows sharply that the highest number of predicates is assigned to the QCS found in the market region: this corresponds to a rich relational condition that brings the QCS to relate with a number of different subjects and to comply with economic rules, legislation, etc., as part of a complex network. Conversely, whenever the QCS is found in a waste dump, its network of relationships is dramatically depleted and the ontological status is diminished. The highest impoverishment occurs when the QCS is thrown away in the environment, so that even the basic information about it is lost. The ethical implications of this state, so well described by the formal language, will not escape the reader.

Table 4: The ontological status of a CS defined on the base of the location of the corresponding QCSs x and the ontological commitments entailed by predicate logic. The flow of information and knowledge between distinct locations is highlighted.

Ontological status	**$\mathfrak{R}$ and knowledge/ information flow**	**Formal definition based on predicate logic**		
Chemical Substance	Chemical lab	$\forall x(P_c(x) \rightarrow (x \in \mathbb{A}))$		(8)
	↕ *Information, knowledge*			
Material	Material science lab	$\forall x((P_c(x) \wedge P_{proc}(x) \wedge P_{perf}(x)) \rightarrow P_{ma}(x))$		(18)
	↕ *Information, knowledge*			
Product	Production plants, packaging, storage	$\forall x ((P_{ma}(x) \wedge P_{pc}(x)) \rightarrow P_P(x))$		(19)
		$\forall x((P_c(x) \wedge P_{proc}(x) \wedge P_{perf}(x) \wedge P_{pc}(x)) \rightarrow P_P(x))$		(20)
	↓ *Information*			
Goods	Market	$\forall x((P_p(x) \wedge P_{cpl}(x) \wedge P_{pur}(x)) \rightarrow P_{go}(x))$		(23)
		$\forall x((P_c(x) \wedge P_{proc}(x) \wedge P_{perf}(x) \wedge P_{pc}(x) \wedge P_{cpl}(x) \wedge P_{pur}(x)) \rightarrow P_{go}(x))$		(24)
	↓ *Information*		$\forall x((P_c(x) \wedge P_{dc}(x) \wedge P_{disp}(x)) \rightarrow P_{lw}(x))$	(25)
Waste	Waste disposal			
		NO Information	$\exists x(P_{disp}(x) \rightarrow P_{iw}(x))$	(26)
		Environment		

The distinct relationships established by quantities of a same CS with distinct regions depend partially on the flow of information and knowledge between regions. We have already clarified that a main difference between information and knowledge lies in the fact that knowledge transfer implies the involvement of human individuals. From this viewpoint, the chemical lab, the material science lab and the production plant appear strictly connected to each other, as researchers and technicians (who bear specific and technical knowledge) are continuously exchanged between working contexts. A well known historical example is provided by the industrial production of polipropilene that required an intense bi-directional exchange between the chemical lab of Giulio Natta, at the Polytechnic University in Milan and the Montecatini industrial plant in Ferrara (Italy) (Cerruti 2013). Interestingly, when products are driven to the market, a radical change occurs: the flow becomes unidirectional and the knowledge transfer mediated by human beings stops. There is only flow of information due to legislation or marketing rules. Table 4 takes for granted that, once the goods are sold, they become objects of current use and all information concerning their usage is lost. This information gap cannot be regimented. When a QCS reappears in the form of waste, two possibilities may occur: the legal and the illegal one. An extremely negative aspect of the illegal way is the complete loss of information as regards the nature of the waste.
All in all, the table shows that, whereas the intrinsic properties of a QCS (i.e. the properties it owns as being part of a CS) are always there, relations are acquired and lost depending on the region $\mathfrak{R}$ where the QCS is placed. The definitions reported in column 3 highlight that – as long as the location of the QCS changes – its relational properties change (they may either improve or be depleted) depending on the network of relationships wherein the QCS is involved.
It is now necessary to reaffirm and clarify the relationship between CS and QCSs. The fact that, in the real world, distinct QCSs of a same CS can display different properties at the same time is evident. Let's take the case of the triple point of a CS, e.g. water, where three phases coexist. In a same location (the triple-point cell) and at a same time, three QCSs of the same CS water instantiate three distinct sets of properties. Note that the triple point is relevant in the definition of the ontological status of a CS, due to its invariance, to the point that van Brakel underlines its possible use as "defining feature" of a pure substance (Van Brakel 2012, p.203). In fact, the whole research activity of chemists is based on the implicit (but crucial) assumption that the results of the manipulation of distinct quantities of a same CS are assignable to the CS as such. Thanks to this assumption, distinct QCSs found and manipulated in different labs may be compared, as they are considered as the instantiation of a same CS in different locations. Our analysis makes explicit that a CS is materially instantiated in a region $\mathfrak{R}$ through a QCS. Hence, the ontological committments referred to a QCS may be extended to the CS of which such quantity represents a fraction. This also leads to the conclusion that the ontological status of a CS is not fully determined by its inherent aspects: it includes a relevant relational contribution. The region may provide meaning and open operational possibilities to the CS as, in distinct regions, distinct relationships are instantiated and the ontological status of the CS is influenced accordingly. Whenever the CS is enriched or deprived of such possibilities, its ontological status is improved or impoverished.

Conclusions

> "*L'idée d'une chose quelconque est l'idée de ses effets sensibles".*
> *"Considérer quels sont les effets pratiques que nous pensons pouvoir être produits par l'objet de notre conception. La conception de tous ces effets est la conception complète de l'objet.*"[22]
>
> Charles Sanders Peirce (1879)

[22] Peirce wrote the French text of "Comment rendre nos idees claires" (Peirce, 1879) in 1875, as 'linguistic exercise' in view of its participation in the meetings of the Permanent Committee of the International Geodetic Association in Paris 20-29 September. Peirce considered the French original of "How To Make Our Ideas Clear" (Peirce, 1878) as the authoritative text for his pragmatic thought (Deledalle, 1981).

According to Pierce, the *effets sensibles* are crucial for defining our conception of a given object. The logical procedure proposed in this work is in line with this viewpoint. Hence an object is affected by a number of *effets pratiques*: a complete understanding of the object's nature has to take into account the ensemble of such effects. This implies that the ontological status of the object is dynamic and reflects the net of relations in which the object is involved. In other words, due to such *effets sensibles,* the object undergoes ontological changes.

This is the thesis underlying the present work. We have chosen to discuss the ontological status of a CS, a central concept in chemistry. In order to do that, we have applied a regimentation procedure based on first-order logic and a locative logic, that are suitable to highlight the implications for distinct quantities of a same CS to be found in different locations at a time.

We believed relevant to formalise through a logical language a usual practice of chemists. Whenever two distinct QCSs are obtained in two different labs and the experimental evidence shows that such QCSs share the very same properties, researchers are led to the general conclusion that such QCSs belong to a same CS, or - in philosophical terms - they consider those QCSs as the instantiation of a same CS. The scientific concept of CS is a formal concept and it is thanks to its formal nature - that overcomes facts such as the presence of impurities or distinct isotopic compositions - that chemists may refer to distinct QCSs as part of a same CS, thus drawing conclusions as regards the properties of the CS as such.

Language is a key issue and the terms employed within a theory are not just the pieces of a semantic interplay: their use implies an ontological commitment. This, in turn, entails a search for simplicity. Quine reminds that "the simplification and clarification of logical theory to which a canonical logical notation contributes is not only algorithmic; it is also conceptual" (Quine 1960, p.161). Forms and contents are intertwined. Regimentation requires seeking for the simplest possible formal expressions.

The sharpness of Table 4 demonstrates the changes occurring in the properties of a CS when it relates to distinct regions. The fact that such changes may be regimented has a relevant implication: as regimentation entails ontological commitments, the formalization through predicate logic allows making explicit and arguing about the relational nature of the ontology of CSs.

As a final remark, we would like to stress that the presence of relational properties has important methodological implications and a strong epistemic relevance, as it highlights the systemic nature of the CS *and* the region wherein it is found. To disjoint CS and region may lead to misinterpretations and loss of information and knowledge about such system.

In conclusion, we believe that the present work complies with Quine's thought when he states that "The quest of a simplest, clearest overall pattern of canonical notation is not to be distinguished from a quest of ultimate categories, a limning of the most general traits of reality" (Quine 1960, p.161).

Acknowledgements

We would like to acknowledge the anonimus reviewer as well as Paul Needham and José Antonio Chamizo for their critical comments on an earlier draft that led us to substantially revise several passages of the manuscript. We do not expect them to agree with the whole of the present work, but their remarks helped us to sharpen our view on this topic. It remains that any flaw that might still be found in the paper is the exclusive responsibility of the authors.

References

Bennett, J. The force of things: Steps toward an ecology of matter. Political theory, 32, 347-372 (2004)

CAS (Chemical Abstract service). http://www.cas.org/content/chemical-substances. Accessed April 14th 2017

Cerruti, L.: Chemicals as Instruments. A Language Game. HYLE-Int.J.Phil.Chem, 4, 39-61 (1998)

Cerruti, L.: Historical and Philosophical Remarks on Ziegler-Natta Catalysts. A Discourse on Industrial Catalysis. HYLE-Int.J.Phil.Chem, 5, 3-41 (1999)

Cerruti, L.: I materiali sintetici: successi, delusioni e speranze. In: V. Marchis, F. Profumo (eds.) Il contributo italiano alla storia del pensiero. Tecnica, pp. 541-552. Istituto della Enciclopedia italiana, Roma (2013).

Chaffee, S. H.: Communication Concepts I: Explication. SAGE, Newbury Park, CA (1991)

Champollion, L., Krifka, M.; Mereology In: Dekker P, Aloni M. (eds), Cambridge Handbook of Semantics, pp.513-541. Cambridge University Press, Cambridge, UK (2015). Available at URL: http://ling.auf.net/lingbuzz/002099. Accessed April 14th 2017

Deledalle, G.: English and French Versions of C. S. Peirce's "The Fixation of Belief and "How To Make Our Ideas Clear", Transactions of the Charles S. Peirce Society 17, 141-152 (1981)

Dumesic, J.A., Huber, G.W., Boudart, M.: Principles of Heterogeneous Catalysis. In: Ertl, G., Knözinger, H., Schüth, F., Weitkamp, J. (Eds.), Handbook of Heterogeneous Catalysis, pp. 1-15. Wiley-VCH Verlag, Weinheim (2008)

ECA (European Chemicals Agency): Guidance in a Nutshell. Identification and naming of substances under REACH and CLP (2011). Available at URL: http://echa.europa.eu/en/support/guidance-on-reach-and-clp-implementation/guidance-in-a-nutshell. Accessed April 14th 2017

Encyclopædia Britannica: Materials processing (2015). Available at URL: http://www.britannica.com/EBchecked/topic/369072/ materials-processing. Accessed April 14th 2017

European Union Commission: Commission Recommendation of 18 October 2011 on the definition of nanomaterial. *Official Journal of the European Union*, L 275/39 (2011). Available at URL: http://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX:32011H0696. Accessed April 14th 2017

Fischer, E.: Einfluss der Configuration auf die Wirkung der Enzyme. Berichte der Deutschen Chemischen Gesellschaft 27, 2985–2993 (1894)

Franklin, B.: Advice to a Young Tradesman, Written by an Old One (1748). Available at URL: https://founders.archives.gov/?q=Advice%20to%20a%20Young%20Tradesman&s=1111311111&r=1. Accessed April 14th 2017

Gabrys, J.: Digital Rubbish a Natural History of Electronics. The University of Michigan Press, Ann Arbor (2013)

Gilmore, C.: Location and Mereology. In Zalta, E.N. (ed.), The Stanford Encyclopedia of Philosophy (2014). Available at URL:

http://plato.stanford.edu/archives/fall2014/entries/location-mereology. Accessed April 14th 2017

Glock, H.-J.: Quine and Davidson on Language, Thought and Reality. Cambridge University Press, Cambridge, UK (2008)
Graham, B.B.: Detail Process Charting: Speaking the Language of Process. John Wiley & Sons, Hoboken, NJ (2004)

Harré, R., Llored, J.-P.: Mereologies as the grammars of chemical discourses. Found. Chemistry. 13, 63-76 (2011)

Hawkins, G.: The Ethics of Waste: How We Relate to Rubbish. University of New South Wales Press, Sydney (2006)

IUPAC: Compendium of Chemical Terminology. Gold Book (2014). Available at URL: https://goldbook.iupac.org/pdf/goldbook.pdf. Accessed April 14th 2017

Kripke, S.: Naming and necessity. In: Davidson, D., Harman, G.H. (Eds.), Semantics of Natural Language, pp. 253–355. Reidel, Dordrech (1972)

Levi, P.: The periodic Table. Schocken Books, New York (1984)

Llored, J.-P.: Chimie, chimie quantique et concept d'emergence: étude d'une mise en relation (2013). Available at URL: https://pastel.archives-ouvertes.fr/pastel-00922954. Accessed April 14th 2017

Llored, J.-P., Harré, R.: Developing the mereology of chemistry. In Calosi, C. and Graziani, P. (Eds.), Mereology and the sciences, pp. 189-212. Springer, Berlin (2014)

McDaniel, K.: Parthood is Identity. In: Kleinschmidt, S. (ed.) Mereology and Location, pp. 13-32. Oxford University Press (2014)

Nature: Homepage of Nature Materials (2015). Available at URL: http://www.nature.com/nmat/authors/index.html#aims-scope. Accessed April 14th 2017

Needham, P.: Modality, Mereology and Substance. In: Woody, A.I., Hendry, R.F., Needham, P. (Eds.) Philosophy of Chemistry, pp. 230-246. North Holland, Oxford (2012a)

Needham, P.: Compounds and Mixtures. In: Woody, A.I., Hendry, R.F., Needham, P. (Eds.) Philosophy of Chemistry, pp. 271-290. North Holland, Oxford (2012b)

Needham, P.: Mereological Structure in Chemical Substances and their Transformations: An Analytic Perspective on the Historical Development of these Concepts. In: Llored, J.P. (Ed.), The Philosophy of Chemistry: Practices, Methodologies, and Concepts, pp. 527-557. Cambridge Scholars Publishing, Newcastle-upon-Tyne, UK (2013)

OECD: Guidance on grouping of chemicals, Series on Testing and Assessment. N.194, p.87. OECD, Paris (2014)

Ohring, M., Gall, D., Baker, S. P.: Materials Science of Thin Films, Third Edition: Deposition and Structure. Academic Press, San Diego (2014)

Peirce, C.S., How To Make Our Ideas Clear. Popular Science Monthly. 12, pp. 286-302 (1878)

Peirce, C.S.: La logique de la science. Deuxiéme partie. Comme rendre nos idées claires. Revue philosophique de la France et de l'étranger. VII, 39-67 (1879).

Polkowski, L.: Approximate Reasoning by Parts. An Introduction to Rough Mereology, Springer, Berlin (2011)

Putnam, H.: Meaning and Reference. J. Philosophy. 70, 699–711 (1973)

Quine, W.V.: The Review of Metaphysics. 2, 21-38 (1948)

Quine, W.V.: Word and Object. MIT Press, Cambridge (Mass.), 2013 (1960)

Quine, W.V.: Philosophy of Logic. Prentice-Hall, New Jersey (1970)

Quine, W.V.: Things and Their Place in Theories. In: Theories and things, pp.1-23. Harvard University Press, Cambridge, MA (1981)

Quine, W. V.: Pursuit of Truth. Harvard University Press, Cambridge, Mass. (1990)

Ryle, G.: The Concept of Mind. The University of Chicago Press, Chicago (1949).

Savjani, K.T., Gajjar, A.K., Savjani, J.K.: Drug Solubility: Importance and Enhancement Techniques. Int. Scholar. Res. Notice. Article ID 195727 (2012).

Sigma Aldrich: On-line catalogue: Lead(II) nitrate (2015). Available at URL: www.sigmaaldrich.com/catalog/product/sial/15194. Accessed April 14th 2017

Spear, A.D.: Ontology for the Twenty First Century: An Introduction with Recommendations. IFOMIS, Saarbrücken, Germany (2006)

Springer, Homepage of the J. Material Science (2015). Available at URL: http://link.springer.com/journal/10853. Accessed April 14th 2017

Taylor, K.: Mottainai: A Philosophy of Waste from Japan, contribute to the meeting on "Philosophy and Waste" held at the Southern Illinois University, November 4-5, 2011. Available at URL: https://philosophyandwaste.files.wordpress.com/2011/10/keving-taylor-siuc.pdf. Accessed April 14th 2017

Van Brakel, J.: The Chemistry of Substances and the Philosophy of MassTerms. *Synthese*, 69, 291-324 (1986)

Van Brakel, J.: Substances: the Ontology of Chemistry. In: Woody, A.I., Hendry, R.F., Needham, P. (Eds.) Philosophy of Chemistry, pp. 191-229. North Holland, Oxford (2012)

Varzi, A.: Mereology. In Zalta, E. N. (ed.), The Stanford Encyclopedia of Philosophy (2014). Available at URL: http://plato.stanford.edu/archives/fall2014/entries/mereology/. Accessed April 14th 2017

Vemulapalli, G.K.: Thermodynamics in Chemistry. In: Woody, A.I., Hendry, R.F., Needham, P. (Eds.) Philosophy of Chemistry, pp. 467-494. North Holland, Oxford (2012)

WHO Expert Committee on Specifications for Pharmaceutical Preparations: General Guidelines for the Establishment, Maintenance & Distribution of Chemical Reference Substances: Annex 3 (2007). Available at URL: http://apps.who.int/medicinedocs/documents/s21438en/s21438en.pdf. Accessed April 14th 2017